

PHASE FIELD METHODS IV

Install-a-Thon / Workshop

NORTHWESTERN UNIVERSITY

CHIMAD.NORTHWESTERN.EDU JANUARY 18th- 20th, 2017



Center for Hierarchical Materials Design (CHiMaD) is a NIST-sponsored center of excellence for advanced materials research focusing on developing the next generation of computational tools, databases and experimental techniques in order to enable the accelerated design of novel materials and their integration to industry, one of the primary goals of the Obama administration's Materials Genome Initiative (MGI).

This Chicago-based consortium includes Northwestern University as the lead, University of Chicago, Northwestern-Argonne Institute for Science and Engineering, a partnership between Northwestern University and Argonne National Laboratory, and the Computational Institute, a partnership between University of Chicago and Argonne National Laboratory. The consortium is also partnered with Questek Innovations, a pioneering materials design company, ASM International and Fayetteville State University.

Designing novel materials of specific properties for a particular application requires simultaneously utilizing physical theory, advanced computational methods and models, materials properties databases and complex calculations. This approach stands in contrast to the traditional trial-and-error method of materials discovery. CHiMaD aims to focus this approach on the creation of novel hierarchical materials which exploit distinct structural details at various scales, from the atomic on up, to obtain enhanced properties. The center's research focuses on both organic and inorganic advanced materials in fields as diverse as self-assembled biomaterials, smart materials for self-assembled circuit designs, organic photovoltaic materials, advanced ceramics and metal alloys.

For more information, please visit chimad.northwestern.edu



Agenda Phase Field Methods IV

Install-a-Thon / Workshop January 18th-20th, 2017 CHiMaD Headquarters

Wednesday, January 18th, 2017

11:45 AM Shuttle from Hilton Garden Inn to CHiMaD HQ

12:00 PM Kick-off lunch

1:00 PM Welcome

Begum Gulsoy

1:05 PM Install-a-Thon (snacks and dinner provided)

Olle Heinonen

9:00 PM Adjourn

Shuttle from CHiMaD HQ to Hilton Garden Inn

Thursday, January 19th, 2017

8:45 AM Shuttle from Hilton Garden Inn to CHiMaD HQ

9:00 AM Breakfast

9:15 AM Attendees present their results of the Install-a-Thon

11:00 AM Coffee break

11:15 AM Discussion of Install-a-Thon results

12:00 PM Lunch

1:30 PM Updates on FiPy and Benchmark I performance

Jonathan Guyer

2:00 PM Updates on MOOSE framework and Benchmark I performance

Daniel Schwen

2:30 PM Updates on PRISMS-PF and Benchmark I performance

Stephen DeWitt

3:00 PM Coffee break

3:15 PM Phase field website

Daniel Wheeler

3:45 PM Current status of benchmark problems

Olle Heinonen, Andrea Jokisaari

4:15 PM Discussion of previous two topics

5:00 PM Reception

7:30 PM Adjourn

Shuttle from CHiMaD HQ to Hilton Garden Inn

Friday, January 20th, 2017

8:30 AM Shuttle from Hilton Garden Inn to CHiMaD HQ

8:45 AM Breakfast

9:00 AM Tutorial on Methods of Manufactured Solutions

Dmitry Karpeyev

9:45 AM MMS lab session

10:45 AM Coffee break

11:00 AM Wrap-up discussion

12:00 PM Adjourn (lunches to-go)

Shuttle from CHiMaD HQ to Hilton Garden Inn

Attendee List Phase Field Methods IV

Install-a-Thon / Workshop January 18th-20th, 2017 CHiMaD Headquarters

Larry Aagesen, Idaho National Laboratory, USA Larry.Aagesen@inl.gov

W. Beck Andrews, University of Michigan, USA wband@umich.edu

Jim Belak, Lawrence Livermore National Laboratory, USA belak1@inl.gov

Amani Cheniour, Pennsylvania State University, USA azc75@psu.edu

Stephen DeWitt, University of Michigan, USA stvdwtt@umich.edu

Begum Gulsoy, Northwestern University/CHiMaD, USA e-gulsoy@northwestern.edu

Jon Guyer, National Institute of Standards and Technology, USA guyer@nist.gov

Olle Heinonen, Argonne National Laboratory, USA heinonen@anl.gov

Andrea Jokisaari, Northwestern University, USA Andrea.jokisaari@northwestern.edu

Trevor Keller, National Institute of Standards and Technology, USA **Trevor.keller@nist.gov**

Mehmet Tumerkan Kesim, University of Connecticut, USA Mehmet.kesim@uconn.edu

Lukasz Kuna, University of Connecticut, USA Lukasz.kuna@uconn.edu

David Montiel, University of Michigan, USA dmontiel@umich.edu

Nana Ofori-Opoku, CHiMaD, National Institute of Standards and Technology, USA Nana.oforiopoku@nist.gov

Bala Radhakrishnan, Oak Ridge National Laboratory, USA

radhakrishnb@ornl.gov

Daniel Schwen, Idaho National Laboratory, USA Daniel.schwen@inl.gov

Pierre-Clement Simon, Pennsylvania Sate University, USA Pjs5523@psu.edu

Peter Voorhees, Northwestern University, USA p-voorhees@northwestern.edu

James Warren, National Institute of Standards and Technology, USA James.warren@nist.gov

Daniel Wheeler, National Institute of Standards and Technology, USA Daniel.wheeler@nist.gov

Phase Field Method IV January 18-20th, 2017

Workshop Location

CHiMaD Headquarters

Northwestern University 2205 Tech Drive Evanston, IL 60208

Parking Information

Please use the North Campus Parking Garage for parking on campus.

If driving, please park at the North Garage, and take a ticket as you enter. Validation tickets will be available at CHiMaD Headquarters.

Hotel & Shuttle Information

Hilton Garden Inn

1818 Maple Ave Evanston, IL 60201 847-475-6400

Hotel Reservations can be made by e-mailing Aquelah.Robinson@Hilton.com

A shuttle is available to and from the workshop, but you are also welcome to walk if you prefer. Please see the map on the next page for locations.

Reimbursements

Please contact Erika Odlaug, Erika.odlaug@northwestern.edu for details.

